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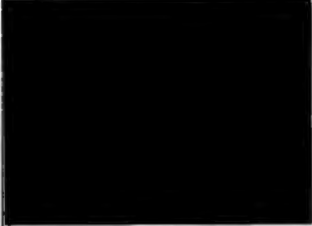
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Health and Safety Research Division

MLSOIL and OSOIL - Computer Codes to Estimate Effective Ground Surface Concentrations for Dose Computations



Computing and Telecommunications Division



Health and Safety Research Division

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HIGHLIGHTS

This report is a user's manual for MLSOIL (Multiple Layer SOIL model) and DFSOIL (Dose Factors for MLSOIL) and a documentation of the computational methods used in those two computer codes. MLSOIL calculates an effective ground surface concentration to be used in computations of external doses. This effective ground surface concentration is equal to (the computed dose in air from the concentration in the soil layers) / (the dose factor for computing dose in air from a plane). MLSOIL implements a five compartment linear-transfer model to calculate the concentrations of radionuclides in the soil following deposition on the ground surface from the atmosphere. The model considers leaching through the soil as well as radioactive decay and buildup. The element-specific transfer coefficients used in this model are a function of the k_d and environmental parameters. DFSOIL calculates the dose in air per unit concentration at 1 m above the ground from each of the five soil layers used in MLSOIL and the dose per unit concentration from an infinite plane source. MLSOIL and DFSOIL have been written to be part of the Computerized Radiological Risk Investigation System (CRRIS) which is designed for assessments of the health effects of airborne releases of radionuclides.

1. INTRODUCTION

This report is a user's manual for MLSOIL (Multiple Layer SOIL model) and DFSoil (Dose Factors for MLSOIL) and a documentation of the computational methods used in those two computer codes. MLSOIL calculates an equivalent ground surface concentration for computation of external doses using available external dose-rate factors (1980). This effective ground surface concentration is equal to (the computed dose in air from the concentration in the soil layers) / (the dose-rate factor for computing dose in air from a plane concentration). MLSOIL uses a five compartment linear-transfer model to calculate the concentrations of radionuclides in the soil resulting from deposition on the ground surface. The model considers leaching through the soil as well as radioactive decay and build-up. The element-specific transfer coefficients used in this model are a function of the k_d and environmental parameters. DFSoil calculates dose-rate factors to determine the dose in air per unit concentration at 1 m above the ground from each of the five soil layers used in MLSOIL and the dose per unit concentration from a surface plane source.

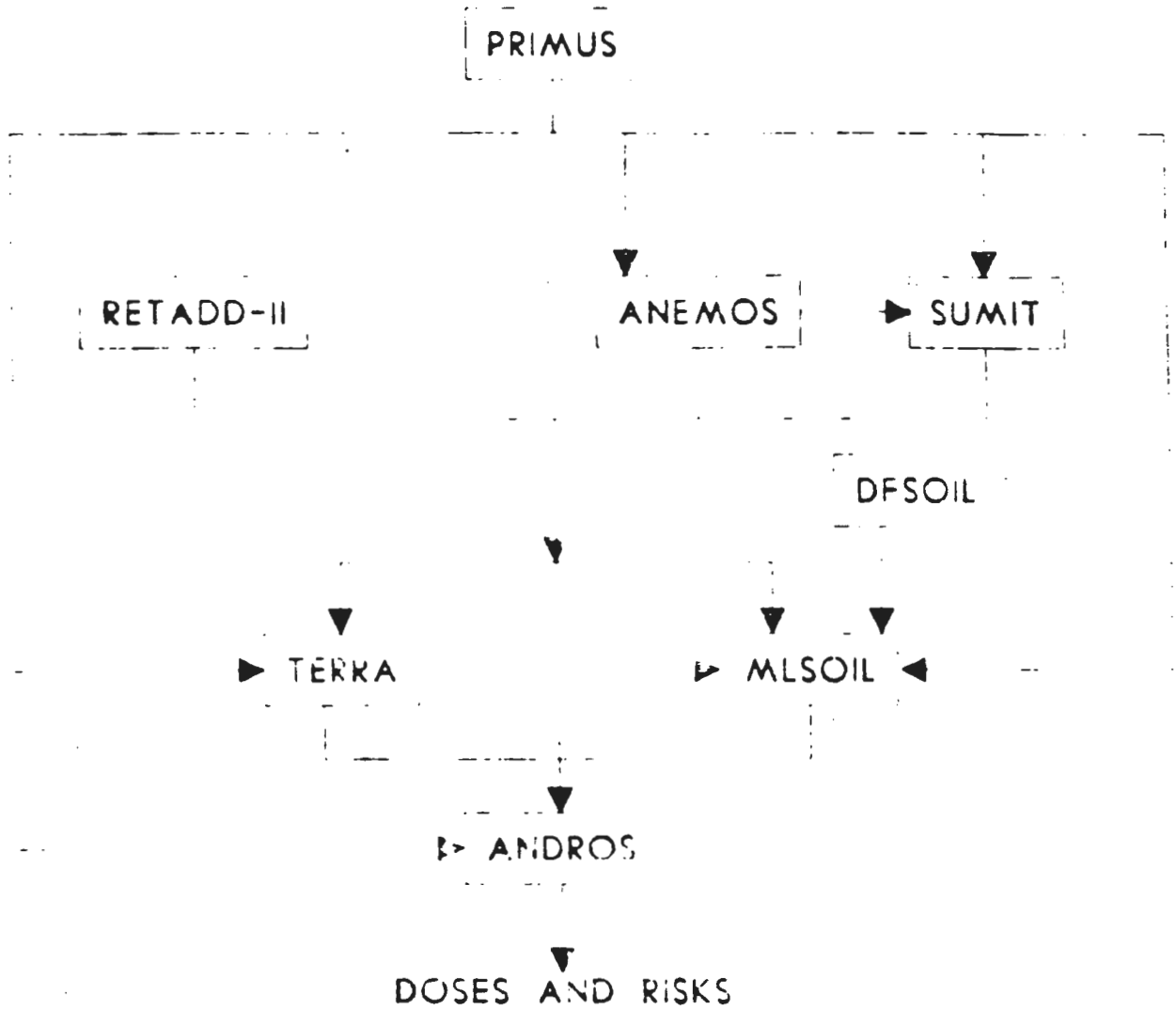
The funding for this research^o was provided by the U.S. Environmental Protection Agency (EPA), which, upon assuming regulatory authority of nuclear effluents covered by the Clean Air Act of 1977, launched an extensive review and revision of models that simulate transport of radionuclides through environmental pathways to man, and calculate resulting health impacts. The results of the first phase of this work, undertaken by the Health and Safety Research Division (HASRD) of the Oak Ridge National Laboratory (ORNL) are published in three

reports: PNEPAR

1979) and DARTAB

DARTAB have provided EPA with an interim methodology for performing nuclear assessments. Work has continued at ORNL on an integrated set of computer codes and data bases which serves as a state-of-the-art radiological risk assessment methodology. This Computerized Radiological Risk Investigation System, or CRRIS (in press), is based on a review and evaluation of the AIRDOS-EPA/DARTAB system. MISOIL and DFSOIL are designed to be an integral part of the CRRIS.

The relationship of MISOIL and DFSOIL to the other codes of the CRRIS is shown in Fig. 1.1. PRIMUS (Hermann et al., in press) accesses a data base of decay data (Kocher, 1981a) to determine the radionuclide decay chains required for the source term which will be considered in transport, dose, and risk calculations by other codes of the CRRIS. RETADD-II (Murphy, Orr, and Begovich, 1984) is a long-range trajectory atmospheric dispersion model which calculates radionuclide air concentrations and ground deposition rates on a square grid on a regional or continental scale. ANEMOS (in press) is a short range (<80km) Gaussian plume atmospheric dispersion model which calculates radionuclide air concentrations and ground deposition rates on a circular grid. Multiple runs of ANEMOS may be summed on a master grid by SUMTJ (Begovich et al., in press). SUMTJ may also be used simply to transform the results from the ANEMOS calculational grid to another grid geometry that is more convenient for the assessment. TLKRA (Baes et al., in press) is used to calculate concentrations of radionuclide chains in four vegetable and produce categories, four cattle feed



1.1. The codes that make up the CHRIS

categories, irrigated and non-irrigated soils, beef, and milk. TERRA uses either RETADD-II, ANEMOS, or user-defined deposition rates. MLSOIL reads deposition rates from RETADD-II, ANEMOS, SUMIT, or TERRA. MLSOIL can either replace TERRA or accept input from that model. MLSOIL will merge its ground surface concentrations with the other environmental concentrations computed in TERRA, if requested. DFSOIL is run to compute the dose-rate factors needed for MLSOIL. ANDROS (Begovich et al., in press) receives environmental radionuclide concentrations from TERRA or MLSOIL and combines them with population estimates, food and air consumption rates, and dose and risk factors to calculate population and average individual doses and risks from the source term supplied to PRIMUS, ANEMOS, or RETADD-II.

MSOIL and DFSOIL were written to provide an alternative to the TERRA methodology for computing dose from ground surface exposure. Estimates of external dose from radionuclides deposited on the ground surface are often based on the assumption that the activity remains on the surface until removed by radioactive decay (USNRC, 1977). For radionuclides deposited on soil, this assumption provides a conservative overestimate of external dose to exposed individuals above ground. Radionuclides will normally be transported downward in soil, e.g., by water infiltration and plowing of agricultural lands. The presence of soil between the source and receptor locations will usually provide much greater shielding than air alone. The method of computing soil activities used in TERRA assumes that there is no contribution to total concentration from radionuclides which have leached below the top 1 cm of soil. Therefore, the external dose computed from the TERRA ground surface concentrations in ANDROS is often underestimated. MLSOIL, using

the dose-rate factors from DFSOIL, computes an effective ground surface concentration that assumes leaching through the top 100 cm of soil. MISOIL and DFSOIL together produce a concentration that can be used to compute a more accurate dose than does TEKRA.

This report documents the models used in MISOIL and DFSOIL and contains instructions for their use. Sect. 2 of this report describes the program MISOIL and the computational methods used in it. Sect. 3 describes the user input to MISOIL in detail and briefly discusses the input files needed. Sect. 4 describes the MISOIL output listing and file. Sect. 5 describes the program DFSOIL. The appendices include listings of MISOIL and DFSOIL, as well as the JCL to run them. Examples of the DFSOIL output report and the MISOIL use, input, and output report are also included in appendices.

2. MISOIL - PROGRAM DESCRIPTION

2.1 Computational Models

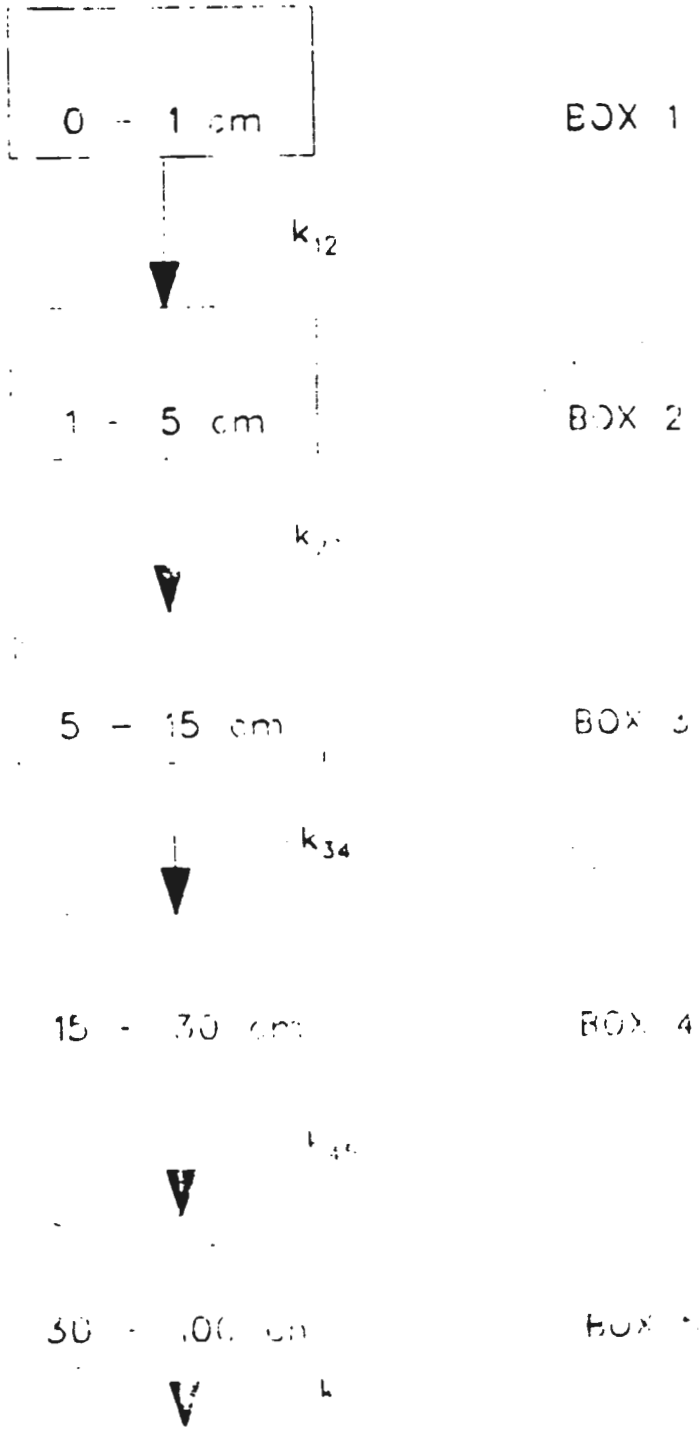
2.1.1 Radionuclide Transport in Soil

The model of radionuclide transport through soil that is implemented in MISOIL is a five compartment linear transfer model. Figure 2.1 shows a schematic of the model which could represent migration through undisturbed agricultural land such as permanent pasture. The movement of radionuclides through the soil column is represented in the model by a series of transfers between compartments of various sizes. Within each compartment the radionuclides are assumed to be uniformly mixed. Note that there is no upward transfer. The rates of transfer between the various compartments are determined by the transfer coefficients k_{ij} . The rate at which this migration takes place is dependent upon several factors, including the compartment thickness, the chemical form of the radionuclide, soil composition, climate, and rainfall. This model is a modification of the model presented by Simmonds, Linsley, and Jones (1979) and used by the Commission of the European Communities (1979).

The rate of change of the activity of radionuclide i in box 1 is given by

$$\frac{dA_1}{dt} = P_1(t) - \lambda_1 A_1 - k_{1,2} A_1 + \sum_j h_{j,1} A_j \quad (2.1)$$

where A_1 (Ci/m^3 or Bq/m^3) is the activity of nuclide in box 1, $P_1(t)$ is the rate at which radionuclide i enters box 1, λ_1 is the radiological



2.1. The soil model used in A. 5011

decay constant for nuclide i . $k_{j,j+1}$ is the leaching removal constant for nuclide i from layer j to layer $j+1$, and $b_{j,i}$ is the branching fraction of nuclide j to nuclide i . Analogous equations can be written for the remaining layers of the model illustrated in Fig. 2.1. The concentrations of all radionuclides in all layers at time t are obtained in MISOIL by solving the set of simultaneous equations represented by Eq. 2.1. Section 2.1.3 describes the method of computing radiologic decay and buildup.

2.1.2 Transfer Coefficients

A leaching removal rate constant model (Bae and Sharp, 1983) has been adapted from the TERRA code (Bae et al., in press) to calculate transfer coefficients in MISOIL. This transfer coefficient is element specific. The model is given by

$$k_{1j} = \frac{P - E}{\theta d [1 + \frac{\rho}{\theta} k_d]} \quad (2.2)$$

where

k_{1j} = the leaching coefficient for element i
between layers j and $j+1$ (s^{-1}),

P = annual average total precipitation (cm/yr),

E = annual average evapotranspiration (cm/yr),

d = thickness of layer j (cm)

ρ = soil bulk density (g/cm^3)

θ = soil volumetric water content (ml/cm^3),

k_d = the distribution coefficient of element i (ml/g).

Migration of radionuclides in soil has been studied only for a limited number of elements, primarily isotopes of cesium, strontium, and plutonium (Simmonds, Linsley, and Jones, 1979). As a result, there is only a very limited empirical data base from which to derive values of the inter-layer transfer coefficients in MISOIL. Computed and measured leaching coefficients for plutonium are compared in Table 2.1. The computed values were obtained from Eq. 2.2, using the default values of ρ and θ (given below), a k_d of 4.0E3 ml/g, and the sum (P-E) equal to the value obtained from the SITE data base for Denver, 52 cm.

In MISOIL as in TERRA, the values of I and E may be entered by the user or read from the SITE data base (Baes et al., 1983b). Annual values of I and E are entered in units of mm and converted to cm. The k_d 's are read from an element-specific file constructed for TERRA. Values of ρ and θ may be entered by the user. The default value for ρ is 1.35 g/cm³. The default value for θ is 0.4895 ml/cm³ (Baes and Sherris, 1983; Baes et al., 1983a). The transfer coefficients may be entered by the user rather than being computed by Eq. 2.2, if desired.

2.1.3 Radioactive Decay and Buildup

The system of equations described by Eq. 2.1 is a system of n linear ordinary differential equations with constant coefficients and constant forcing term. This system can be expressed as a vector matrix differential equation

$$\frac{dA}{dt} = (A - P) + C_0 \quad (2.3)$$

subject to the initial condition

Table 2.1 A comparison of plutonium leaching coefficients

Layer (cm)	Measured ^a (yr ⁻¹)	Computed (yr ⁻¹)
0-1	2.43E-1	8.57E-3
1-5	6.29E-2	2.14E-3
5-15	3.92E-2	8.57E-4
15-30	1.47E-3	5.71E-4

^afrom Simmonds, Linsley, and Jones (1979).

$$A(t_0) = A_0. \quad (2.4)$$

In our notation, A is a vector function of t , A_0 and P are constant vectors, and C is a constant coefficient matrix. A is a vector of the nuclide activities, P is a vector of the deposition rates, and C is the matrix of coefficients of the differential equations, including decay and inter-layer transfer factors.

The unique solution of the system Eqs. 2.3 - 2.4 is

$$A(t) = \exp[(t-t_0)C]A_0 + \int_{t_0}^t \exp[(t_0-\tau)C]P \, d\tau, \quad (2.5)$$

where $\exp(\)$ means the matrix exponential function of order n (Coddington and Levinson, 1955).

For values of $(t-t_0)C$ for which the matrix norm $\|[(t-t_0)C]\|$ is large, direct application of Eq. 2.5 is not practical for numerical evaluation of $A(t)$. However a series method has been developed for a suitably rearranged version of Eq. 2.5; this method has been applied to radioactive decay processes for some time and is discussed by Lee (1976), whose report is the primary basis for our adaptation. We proceed to describe the method and our application of it.

We define the matrix function $D(S)$ as follows:

$$D(S) = \sum_{i=1}^{\infty} \frac{S^i}{(i+1)!}. \quad (2.6)$$

where S is a matrix. The series converges for all S , and hence $D(S)$ is well-defined. In the special case where L is nonsingular,

$$A(t_0) = A_0. \quad (2.4)$$

In our notation, A is a vector function of t , A_0 and P are constant vectors, and C is a constant coefficient matrix. A is a vector of the nuclide activities, P is a vector of the deposition rates, and C is the matrix of coefficients of the differential equations, including decay and inter layer transfer factors.

The unique solution of the system Eqs. 2.3 - 2.4 is

$$A(t) = \exp\left\{(t-t_0)C\right\}A_0 + \int_{t_0}^t \exp\left[(t_0-\tau)C\right]P d\tau, \quad (2.5)$$

where $\exp\{\dots\}$ means the matrix exponential function of order n (Goldington and Levinson, 1955).

For values of $(t-t_0)C$ for which the matrix norm $\| (t-t_0)C \|$ is large, direct application of Eq. 2.5 is not practical for numerical evaluation of $A(t)$. However a series method has been developed for a suitably rearranged version of Eq. 2.5; this method has been applied to radioactive decay processes for some time and is discussed by Lee (1966), whose report is the primary basis for our adaptation. We proceed to describe the technique and our application of it.

We define the matrix function $D(S)$ as follows

$$D(S) = I + \sum_{k=1}^{\infty} \frac{S^k}{k!} \quad (2.6)$$

where S is a matrix. The series converges for all S , and hence $D(S)$ is well defined in the special case where S is nonsingular.

$$D(S) = S^{-1}(\exp(S) - I) , \quad (2.7)$$

where I is the identity matrix. With

$$S = (t-t_0)C , \quad (2.8)$$

it is possible to use Eqs. 2.5, 2.6, and 2.7 to prove that

$$A(t) = [SD(S)+I]A_0 + (t-t_0)D(S)P . \quad (2.9)$$

Application of Eq. 2.6 to the numerical evaluation of $D(S)$ in Eq. 2.9 depends on a scaling operation that transforms S to a matrix with eigenvalues less than one in magnitude and thus accelerates the convergence of the series. The scaling is defined by the equation

$$H = 2^{-p}S , \quad (2.10)$$

where p is a positive integer, chosen so that the eigenvalues of H are less than one in absolute value (each eigenvalue of H is 2^{-p} times an eigenvalue of S). If we assume for the moment that such a value of p is known, then computation of $D(S)$ for substitution in Eq. 2.9 breaks down to the following steps:

Step 1. Compute H from Eq. 2.10 and $D(H)$ from the approximate formula

$$D(H) = \sum_{i=1}^M \frac{H^i}{(i+1)!} = I + \frac{1}{2}H + \dots + \frac{1}{M} \left(H \left(I + \frac{1}{1+M}H \right) \dots \right) , \quad (2.11)$$

where M can be estimated to give a prescribed accuracy.

Step 2. Using the computed value from Eq. 2.11 in the recursion formula

$$D(2^k H) = D(2^{k-1} H) \left(I + \frac{1}{2} (2^{k-1} H) D(2^{k-1} H) \right), \quad k = 1, 2, \dots, p. \quad (2.12)$$

compute $D(2^p H) = D(S)$.

Step 3. Substitute $D(S)$ into Eq. 2.9 to get $A(t)$.

A value of p such that the transformation in Eq. 2.10 produces a matrix H with eigenvalues less than unity in magnitude may be determined from the inequality

$$p > \ln \left(\sum_{j=1}^n \sum_{i=1}^n s_{ij}^2 \right) / (2 \ln 2), \quad (2.13)$$

where s_{ij} is the (i, j) -th entry of the matrix S . This inequality is the result of the following considerations:

1. The eigenvalues $\mu_i, i = 1, \dots, n$, of $H^T H$ are real and nonnegative, and

$$\max_i |\lambda_i| < \max_i \mu_i, \quad (2.14)$$

where the λ_i are the eigenvalues of H (Weyl's inequality; see Gantmacher (1959), footnote on p. 277, for references).

2. If $H = [h_{ij}]$, then

$$\text{trace}(H^T H) = \sum_{i=1}^n \sum_{j=1}^n h_{ij}^2 = \sum_{i=1}^n \mu_i. \quad (2.15)$$

The first inequality follows from a direct computation; the second is a consequence of the fact that the trace of a matrix is invariant under similarity transformations, and $\sum_{i=1}^n u_i$ is the trace of the Jordan canonical form of $H^T H$.

3. By combining Eqs. 2.14 and 2.15, we see that

$$\max_i |\lambda_i|^2 \left(\sum_{i=1}^n h_{ij}^2 \right) = \sum_{i=1}^n \sum_{j=1}^n h_{ij}^2 = \sum_{j=1}^n \sum_{i=1}^n (2^{-p} s_{ij})^2. \quad (2.16)$$

It follows from Eq. 2.16 that we may enforce the condition $|\lambda_i| < 1$ for $i = 1, \dots, n$ by requiring that

$$\left[\sum_{j=1}^n \sum_{i=1}^n s_{ij}^2 \right]^{\frac{1}{2}} < 2^p. \quad (2.17)$$

Inequality 2.17 is equivalent to Eq. 2.13.

The matrix C and the vectors A and P are constructed as follows. The vectors A and P are partitioned into N blocks, one block per nuclide, with each block containing five components, one for each soil layer. The initial value of A is always zero. If the period of long-term buildup (t_b) is greater than or equal to the assessment period (t_a), the activities are computed with the entered constant deposition rate for the whole assessment period. If $t_a > t_b$ the set of equations must be solved twice, first, for t_b with the entered constant deposition rate and, second, for $(t_a - t_b)$ with both a zero deposition rate and an initial activity as computed for the period of long-term buildup (t_b).

The coefficient matrix C is partitioned into an $N \times N$ array of submatrix blocks, each of which is 5×5 . The submatrix block for each nuclide pair (i,j) is defined as follows:

for $j > i$ as the 0 matrix, (2.18)

for $j < i$ as $\lambda_i b_{i,j} I$,

for $j = i$ as

$$\begin{array}{ccccc} -\lambda_i - k_{i,1} & 0 & 0 & 0 & 0 \\ k_{i,1} & -\lambda_i - k_{i,2} & 0 & 0 & 0 \\ 0 & k_{i,2} & -\lambda_i - k_{i,3} & 0 & 0 \\ 0 & 0 & k_{i,3} & -\lambda_i - k_{i,4} & 0 \\ 0 & 0 & 0 & k_{i,4} & -\lambda_i - k_{i,5} \end{array}$$

with

I being the 5×5 identity matrix

λ_i being the radiologic decay constant of nuclide i ,

$k_{i,m}$ being the transfer coefficient of nuclide i
from layer m to layer $m+1$,

$b_{i,j}$ being the branching fraction of nuclide i to nuclide j .

The λ_i 's and $b_{i,j}$'s are from PRIMUS. The $k_{i,j}$'s are computed in routine TRANSF or entered by the user. Note that the matrix C is lower triangular.

2.2 Introduction to the Code

MLSOIL has been written to function in the same position within the ORRIS as does TERRA. Because of this, several routines were taken from TERRA and modified for use in MLSOIL. These are the TERRA main routine

Table 3.3 K_d 's used in MLSOIL

element	K_d ml/g	element	K_d ml/g
AC	1.5E+03	N	5.0E-01
AG	4.5E+01	NA	1.0E+02
AL	1.5E+03	NB	3.5E+02 ✓
AM	7.0E+02 ✓	ND	6.5E+02
AS	2.0E+02	NI	1.5E+02 ✓
AT	1.0E+01	NP	3.0E+01 ✓
AU	2.5E+01	OS	4.5E+02
B	3.0E+00	P	3.5E+00
BA	6.0E+01	PA	2.5E+03 ✓
BE	6.5E+02	PB	9.0E+02 ✓
BI	2.0E+02	PD	6.0E+01 ✓ Doc 10
BR	7.5E+00	PH	6.5E+02
CA	4.0E+00 ✓	PO	5.0E+02
CD	6.5E+00	PK	6.5E+02
CE	8.5E+02	PT	9.0E+01
CI	2.5E-01 ✓	PU	4.5E+03 ✓
CM	2.0E+03 ✓	RA	4.5E+02 ✓
CO	4.5E+01	RB	6.0E+01 ✓
CR	8.5E-02	RE	7.5E+00
CS	1.0E+03 ✓	RI	6.0E+01
CU	3.5E+01	RU	3.5E+02
DY	6.5E+02	S	7.5E+00
ER	6.5E+02	SH	4.5E+01
EU	6.5E+02	SC	1.0E+03
F	1.5E+02	SE	3.0E+02 ✓ Se 10
FE	2.5E+01	SI	3.0E+01
FR	2.5E+02	SP	6.5E+01
GA	1.5E+03	SN	2.5E+02 ✓
GD	6.5E+02	SR	3.5E+01 ✓
GE	2.5E+01	TA	6.5E+02
HF	1.5E+03	TB	6.5E+02
HC	1.0E+01	TC	1.5E+00 ✓ TC 10
HO	6.5E+02	TE	3.0E+02
I	6.0E+01 ✓	TH	1.5E+05
IN	2.5E+03	TI	1.0E+03
IK	1.5E+02	TL	1.5E+03
K	5.5E+00	TM	6.5E+02
LA	6.5E+02	U	4.5E+02 ✓
LI	3.0E+02	V	1.0E+03
LU	6.5E+02	W	1.5E+02
MA	4.5E+00	Y	5.0E+02
MB	6.5E+01	YB	6.5E+02
MC	2.0E+01 ✓	Zn	4.0E+01
		Zk	5.0E+03 ✓

I $K_d = 100$ if $K_d = 100$

5. DFSOIL

5.1 Introduction

DFSOIL calculates the external dose-rate factors in air for photon sources in soil and for photon sources on the ground plane. The dose-rate factors for soil layers are computed for specific soil layer thicknesses and specific nuclides. These dose-rate factors are intended to be used in environmental dose assessments, particularly in MISOIL. The soil calculations represent an extension of previous calculations for photon sources which are confined to the ground surface

in that the source concentration at a given depth in soil is assumed to be uniform over an infinite plane surface parallel to the ground. With this assumption, the external dose rate \dot{H} at any time t to an exposed individual can be expressed in the general form

$$\dot{H}(t) = A(t) \times DRF, \quad (5.1)$$

where A is the radionuclide concentration at the location of the exposed individual and DRF denotes the dose-rate conversion factor, which we also call the dose-rate factor, defined by this equation as the dose rate per unit source concentration. The concept of the external dose-rate conversion factor is discussed in more detail elsewhere

For the purposes of this computation, we note only that the dose-rate factor for external exposure to photon emitters on the ground surface depends on the height

of the receptor location above ground, which is usually assumed to be 1 m. For photon emitters in soil, however, the dose-rate factor depends on the depth in soil but is usually insensitive to the height of the receptor location above ground for locations near the ground surface.

External dose from electron emitters in soil is not considered here. For electrons produced by radioactive decay, the electron range in soil is usually less than 2 cm and never exceeds 4 cm (NAS, 1964). Therefore, a nominal penetration of radionuclides into soil will provide complete shielding from all electron radiations.

5.2 Computation of Dose-Rate Factors

This section presents calculations of photon dose-rate factors in air above ground for monoenergetic sources at various depths in soil and on the ground plane. The calculations assume that the source concentration is uniform over a horizontal plane.

An equation for the dose-rate factor in air for monoenergetic photon sources which are confined to the ground surface has previously been derived (Kocher, 1980; Kocher, 1981; Kocher, 1983a). The result is

$$DRF_{\gamma}^a(z, E_{\gamma}) = \frac{1}{2} K E_{\gamma} (\mu_{en}/\rho)_a \left[E_1(\mu_a z) - \frac{C_a}{(D_a - 1)} \exp[(D_a - 1)\mu_a z] \right] \quad (5.2)$$

Here, DRF_{γ}^a is the photon (γ) dose-rate factor in air (a) in units of Gy/sec per Bq/m²; z is the height of the receptor location above ground in cm; E_{γ} is the photon energy in MeV; K is a constant equal to the product of 1.6×10^{-10} g-Gy/McV and 10^{-4} cm²/m²; $(\mu_{en}/\rho)_a$ and μ_a are the mass energy-absorption and linear attenuation coefficients in air in

units of cm^2/g and cm^{-1} , respectively, for energy E_γ ; C_a and D_a are the coefficients in the Berger form of the energy-absorption buildup factor in air for energy E_γ (B_{on}^a) given by ([redacted] 1966)

$$B_{\text{on}}^a = 1 + C_a \mu_a r - \exp(D_a \mu_a r) \quad (5.3)$$

where r is the distance from any point in the source region to the receptor position; and \tilde{E}_1 is the first-order exponential integral

$$\tilde{E}_1(\mu_a z) = \int_z^\infty \frac{1}{r} \exp(-\mu_a r) dr \quad (5.4)$$

For an exposed individual standing on the ground, the dose-rate factor is usually calculated for the single height $z = 1$ m above ground.

The dose-rate factors for monoenergetic sources are applied to radionuclides by assuming that the spectrum of photons from radioactive decay consists of discrete γ and X rays. Therefore, the dose-rate factor for ground-surface exposure to a particular radionuclide DRF_γ^g is given by

$$\text{DRF}_\gamma^g(z) = \sum_i f_{i\gamma} \text{DRF}_\gamma^a(z, E_{i\gamma}) \quad (5.5)$$

where $f_{i\gamma}$ is the intensity of the i th photon of energy $E_{i\gamma}$ in number per decay and the summation includes all photons in the decay spectrum.

The dose-rate factor in air for monoenergetic sources in soil can be obtained by analogy with Eq. 5.2 by calculating photon attenuation

and buildup in soil rather than in air. Thus the dose-rate factor in air immediately above the soil layer as a function of depth x of the monoenergetic plane source in soil is given by

$$DRF_{\gamma}^a(x, E_{\gamma}) = \frac{1}{2} \frac{K_{\gamma}}{E_{\gamma}} (\mu_{en}/\rho)_a \left[\bar{E}_1(118x) - \frac{C_1}{(D_s - 1)} \exp[(D_s - 1)\mu_s x] \right] \quad (5.6)$$

Note that even though the medium between the source and receptor positions is assumed to be in soil rather than in air, we are still calculating the dose-rate factor at a receptor location in air. Thus the dose-rate factor itself and the mass-energy absorption coefficient on the right hand side of Eq. 5.6 are values in air and not in soil.

In practice, Eq. 5.6 is to be evaluated at 1 m above ground, and not immediately above ground. The effect of the layer of air between the soil surface and the receptor can be approximated by a layer of soil which would provide the same shielding as the layer of air. This equivalent depth of soil, x_a , may be calculated by setting Eq. 5.6 equal to Eq. 5.2 and solving the resulting transcendental equation for x_a . For $x = 1$ m, the resulting value of x_a is less than 1 mm for all photon energies. The dose-rate factor for a receptor 1 m above the soil surface may then be calculated for a plane monoenergetic source at a depth x by evaluating Eq. 5.6 at $x+x_a$ rather than at x . For all practical purposes, however, it is clear that x_a can be neglected compared with the depth x in soil; i.e., the layer of air above ground contributes little to photon shielding from sources in soil.

The mass energy absorption and linear attenuation coefficients in air used in Eqs. 5.2 and 5.6 were obtained from the compilation by

Bubbell (1969). The buildup factor coefficients in (5.6) were obtained from a linear least-squares fit of Eq. 5.3 to published energy-absorption buildup factors (Bubbell 1969). The parameters for photon transport in soil were obtained by assuming that available data for concrete are appropriate. The linear attenuation coefficients and the coefficients for the energy-absorption buildup factor for concrete were obtained from the calculations of Eisenbauer and Simmons (1975); the former assume a soil density of 1.4 g/cm^3 .

Radionuclides in soil will usually be distributed throughout a volume rather than confined to a plane surface. The dose rate in air above ground from a volume source can be obtained by an integration of the plane-source dose-rate factor and the radionuclide concentration over the source volume. From Eq. 5.1, the dose rate in air, \dot{H}_Y^a , for energy E_Y is given by

$$\dot{H}_Y^a(E_Y) = \int_{x_1}^{x_2} A_s(x) \text{DKF}_Y^a(x+x_0, E_Y) dx, \quad (5.7)$$

where $A_s(x)$ is the source concentration at depth x in Bq/v^3 and x_1 and x_2 are the upper and lower boundaries of the source region, respectively, and x_0 is the thickness of soil corresponding to 1 m of air as discussed following Eq. 5.6. Again, x_0 can usually be neglected in practical applications, because the value is less than 1 mm.

For most distributions of sources with depth in soil, Eq. 5.7 must be solved numerically. The dose-rate factor for a slab source is obtained by integrating Eq. 5.6 over the vertical extent of the slab, using the relation for derivatives of exponential integrals (Gattachi and Cahill, 1965),

$$d\tilde{E}_n(\omega)/d\omega = -\tilde{E}_{n-1}(\omega) \quad (5.8)$$

the result is

$$\begin{aligned} DRF_{\gamma}^n(x_1, x_2, E_{\gamma}) &= \frac{1}{2} \Delta E_{\gamma} (\mu_{eff}/\nu)_{\alpha} \frac{1}{\mu_{\alpha}} E_2(\mu_{\alpha} x'_1) - \tilde{E}_2(\mu_{\alpha} x'_2) \\ &\cdot \frac{C_{\alpha}}{(D_{\alpha} - 1)^2} \left[\exp[(D_{\alpha} - 1)\mu_{\alpha} x_1] - \exp[(D_{\alpha} - 1)\mu_{\alpha} x_2] \right] \end{aligned} \quad (5.9)$$

where the dose rate factor in air is in units of Gy/sec per Bq/m^3 and the second-order exponential integral is given by (Gautschi and Cahill, 1965)

$$\tilde{E}_2(\omega) = \exp(-\omega) - \omega \tilde{E}_1(\omega) \quad (5.10)$$

The variables x'_1 and x'_2 are equal to $x_1 + x_0$ and $x_2 + x_0$, respectively. Again, x_0 can usually be neglected. The nuclear-specific dose-rate factors for slab sources are computed by summing these monoenergetic factors analogously to Eq. 5.5, as

$$DRF_{\gamma}^n(x_1, x_2) = \sum_{\alpha} I_{\alpha} DRF_{\gamma}^n(x_1, x_2, E_{\alpha\gamma}) \quad (5.11)$$

6. SUMMARY

MLSOIL and DFSOIL will be useful in producing radiation doses from ground surface exposures. MLSOIL computes an effective ground surface concentration as the ratio of the dose from a five-layer soil model to the dose-rate factor for computing dose from the ground plane. DFSOIL computes the dose-rate factors needed in DFSOIL for the five soil layers and for the ground plane.

MLSOIL and DFSOIL were written to be used as an integral part of the CRRIS or with other compatible codes available to the user. MLSOIL and DFSOIL do not compute doses to the body or organs by themselves. MLSOIL can print the dose in air from ground surface exposure, so that ANDROS need not be run if that is the only dose of interest. If the output file of DFSOIL is available, there is no need to rerun DFSOIL. MLSOIL can be run with a variety of options within the CRRIS to produce ground surface concentrations, which may be combined with other environmental concentrations from TERRA, and entered to ANDROS for computation of the needed doses and risks.

7. REFERENCES

- [1] C. F. Baes III and R. D. Sharp. 1983. "A Proposal for Estimation of Soil Leaching and Leaching Constants for Use in Assessment Models", in J. Environ. Qual., 12, 17.
- [2] C. F. Baes, III, C. W. Miller, B. D. Murphy, and A. L. Sjoreen. In press. An Introduction to CHAS. A Computerized Radiological Risk Investigation System for Assessing Atmospheric Release of Radionuclides. ORNL/TM 8573
- [3] C. F. Baes III, R. D. Sharp, A. L. Sjoreen, and O. W. Bergmann. In press a. TERKA. A Computer Code for Calculation of the Damages of Environmentally Released Radionuclides Through Agriculture. ORNL 5785.
- [4] C. F. Baes III, R. D. Sharp, A. L. Sjoreen, and R. W. Shor. In press b. A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides Through Agriculture. ORNL-5786.
- [5] C. L. Begovich, H. F. Polerman, E. C. Schlatter, S. Y. Obr, and K. G. Chester. 1981. DARTAB: A Program to Combine Airborne Radionuclide Environmental Exposure Data with Dosimetric and Health Effects Data to Generate Tabulations of Predicted Health Impact. ORNL-5692.
- [6] C. L. Begovich, N. J. Dellich, J. T. Holdeman, Jr., A. L. Sjoreen, and C. W. Miller. In press. PUMIT. A Computer Code to

Interpolate and Sum Single Kelesse Atmospheric Model Results onto a Master Grid. ORNL-5914.

- [7] C. L. Begovich, S. Y. Ohr, A. L. Sjoreen, and R. O. Chester. In press. ANDROS: A Code for Assessment of Nuclide Doses and Risks with Option Selection. ORNL-5889.
- [8] F. A. Coddington and N. Levinson. 1955. Theory of Ordinary Differential Equations. McGraw-Hill Book Co., Inc., New York.
- [9] Commission of the European Communities. 1979. Methodology for Evaluating the Radiological Consequences of Radioactive Effluents Released in Nuclear Operations. Doc. No. V/3605/79-LN,FK.
- [10] A. H. Chilton. 1968. "Broad Beam Attenuation", in: Engineering Compendium on Radiation Shielding. Vol. I (Edited by R. G. Jaeger), p. 202 (New York: Springer-Verlag).
- [11] F. H. Clark. 1969. "Gamma-Ray Buildup Factors for Sand, Air, and Wood (Cellulose)". Nucl. Appl. 6, 588.
- [12] D. E. Dunning, Jr., E. W. Leggett, and N. G. Yalcintas. 1980. A Combined Methodology for Estimating Dose Rates and Health Effects from Radioactive Pollutants. ORNL/TM-7105.
- [13] C. M. Eisenhauer and G. L. Simms. 1975. "Point Isotropic Gamma-Ray Buildup Factors in Concrete" Nucl. Sci. Eng. 56, 263.
- [14] F. R. Gantmacher. 1959. Matrix Theory. Vol. 1. Chelsea Publishing Co., Inc., New York.

- [15] W. Gautschi and W. F. Cahill. 1965. "Exponential Integral and Related Functions", in: Handbook of Mathematical Functions, (Edited by M. Abramowitz and E. A. Stegun). p. 227 (New York: Dover Press).
- [16] O. W. Hermann, C. F. Baes III, C. W. Miller, C. L. Begovich, and A. L. Sjoreen. In press. PHIMUS. A Computer Code for the Preparation of Radionuclide In-growth Matrices from User-specified Sources. ORNL-5912.
- [17] J. H. Hubbell. 1969. Photon Cross Sections, Attenuation Coefficients, and Energy Absorption Coefficients from 10 keV to 100 GeV. National Bureau of Standards Report NSRDS-NBS 29 (Washington, D. C.: U.S. Department of Commerce).
- [18] D. C. Kocher. 1980. "Dose-Rate Conversion Factors for External Exposure to Photon and Electron Radiation from Radionuclides Occurring in Routine Releases from Nuclear Fuel Cycle Facilities". Health Phys. 25, 543.
- [19] D. C. Kocher. 1981a. Radionuclide Decay Data Tables. U. S. Department of Energy, DOE/TIC-11026.
- [20] D. C. Kocher. 1981b. Dose-Rate Conversion Factors for External Exposure to Photons and Electrons. NUREG/CR-1918. ORNL/NUREG-79.
- [21] D. C. Kocher. 1983a. "Dose-Rate Conversion Factors for External Exposure to Photons and Electrons". Health Phys., in press.

- [22] D. C. Kocher. 1983b. "External Dosimetry", in: Radiological Assessment (Edited by J. E. Till and H. R. Meyer), Chap. 6 (Washington, D. C.: U.S. Nuclear Regulatory Commission).
- [23] C. E. Lee. 1976. The Calculation of Isotopic Mass and Energy Production by a Matrix Operator Method. LA-6483-MS.
- [24] C. W. Miller, C. L. Begovich, O. W. Hermann, and A. L. Sjoreen. In press. ANEMOS: A Computer Code to Estimate Air Concentrations and Ground Deposition Rates for Atmospheric Nuclides Emitted from Multiple Operating Sources. ORNL-5913.
- [25] R. E. Moore, C. F. Bacs III, L. M. McDowell-Boyer, A. P. Watson, F. O. Hoffman, J. C. Pleasant, and C. W. Miller. 1979. AIRDOS-EPA: A Computerized Methodology for Estimating Environmental Concentrations and Dose to Man from Airborne Releases of Radionuclides. ORNL-5532.
- [26] B. D. Murphy, S. Y. Ohr, and C. L. Begovich. In press. RETADD-II: A Long Range Atmospheric Trajectory Model with Consistent Treatment of Deposition Loss and Species Growth and Decay. ORNL/CSD-99.
- [27] National Academy of Sciences-National Research Council. 1964. Studies in Penetration of Charged Particles in Matter. Publication 1133 (Washington, D. C.: National Academy of Sciences).

- [28] J. P. Diamonds, G. S. Linsley, and J. A. Jones. 1979. A General Model for the Transfer of Radioactive Materials in Terrestrial Food Chains. National Radiological Protection Board, Harwell, Didcot, Oxon, England, NRPB-R89.
- [29] A. L. Sjoreen and C. W. Miller. 1984. TRIPAR - A User-Friendly Preprocessor to Create AIMS-EPA Input Data Sets. ORNL-5952.
- [30] D. K. Trubey. 1966. A Survey of Empirical Functions Used to Fit Gamma Ray Building Factors. Oak Ridge National Laboratory, Oak Ridge, TN, ORNL-NSIC-10.
- [31] U. S. Nuclear Regulatory Commission. 1977. Regulatory Guide 1.109. Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50 Appendix I (Revision 1). Office of Standards Development.